

10/751, 388

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 10:47:02 ON 13 JUL 2007

FILE 'REGISTRY' ENTERED AT 10:47:13 ON 13 JUL 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 JUL 2007 HIGHEST RN 942260-92-6
DICTIONARY FILE UPDATES: 12 JUL 2007 HIGHEST RN 942260-92-6

New CAS Information Use Policies. enter HELP USAGETERMS for details.

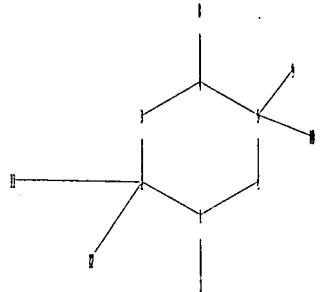
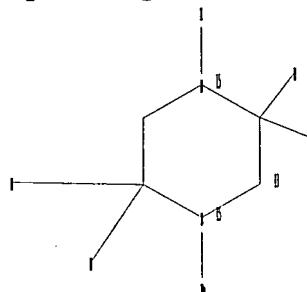
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

```
=> Uploading C:\Program Files\Stnexp\Queries\10751388.str
```



```

chain nodes :
7 8 9 10 11 12
ring nodes :
1 2 3 4 5 6
chain bonds :
1-7 2-11 2-12 4-
ring bonds :
1-2 1-6 2-3 3-4
exact/norm bonds :

```

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1-2 1-6 2-3 3-4 4-5 5-6
exact bonds :
1-7 2-11 2-12 4-8 5-9 5-10

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> s 11
SAMPLE SEARCH INITIATED 10:47:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 69561 TO ITERATE

2.9% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1375516 TO 1406924
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> scr 2039
L3 SCREEN CREATED

=> s 11 and 13
SAMPLE SEARCH INITIATED 10:48:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 192 TO ITERATE

100.0% PROCESSED 192 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3009 TO 4671
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L1 AND L3

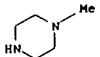
=> s 11 and 13 full
FULL SEARCH INITIATED 10:48:58 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3784 TO ITERATE

100.0% PROCESSED 3784 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L5 4 SEA SSS FUL L1 AND L3

=> d 15 1-4

L5 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 877154-66-0 REGISTRY
 ED Entered STN: 17 Mar 2006
 CN Piperazine, 1-methyl-, labeled with deuterium (9CI) (CA INDEX NAME)
 MF C5 H8 D4 N2
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER
 IL 4H-2



1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 791743-80-1 REGISTRY
 ED Entered STN: 02 Dec 2004
 CN Piperazine, 1-methyl-, labeled with carbon-13 (9CI) (CA INDEX NAME)
 MF C5 H12 N2
 CI COM
 SR CA
 IL XC-13



L5 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 119550-27-5 REGISTRY
 ED Entered STN: 10 Mar 1989
 CN Piperazine, 1-methyl-, labeled with tritium (9CI) (CA INDEX NAME)
 MF C5 H12 N2
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT
 IL XH-3



1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 112023-61-7 REGISTRY
 ED Entered STN: 25 Dec 1987
 CN Piperazine, 1-methyl-, labeled with carbon-13, dihydrochloride (9CI) (CA INDEX NAME)
 MF C5 H12 N2 . 2 Cl H
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
 IL XC-13
 CRN (791743-80-1)



●2 HCl
 1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	181.70	181.91

FILE 'CAPLUS' ENTERED AT 10:50:00 ON 13 JUL 2007
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FILE COVERS 1907 - 13 Jul 2007 VOL 147 ISS 4
FILE LAST UPDATED: 12 Jul 2007 (20070712/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> d his

(FILE 'HOME' ENTERED AT 10:47:02 ON 13 JUL 2007)

FILE 'REGISTRY' ENTERED AT 10:47:13 ON 13 JUL 2007
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 SCR 2039
L4 0 S L1 AND L3
L5 4 S L1 AND L3 FULL

FILE 'CAPLUS' ENTERED AT 10:50:00 ON 13 JUL 2007

=> s 15
L6 3 L5

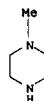
=> d ibib abs hitstr 1-3

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:619662 CAPLUS
 DOCUMENT NUMBER: 144:254085
 TITLE: Syntheses of [¹⁴C] and [²H]PD0205520, an inhibitor
 of the tyrosine kinase activity of the epidermal growth
 factor receptor
 AUTHOR(S): Zhang, Yingsheng; Huang, Yun; Huang, Che C.
 CORPORATE SOURCE: Radiochemistry Group, Chemical R&D, Michigan
 Pharmaceutical Sciences, Pfizer Inc., Kalamazoo, MI,
 49007, USA
 SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals
 (2005), 48(7), 485-496
 CODEN: JLCRD4; ISSN: 0362-4803
 PUBLISHER: John Wiley & Sons Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:254085
 AB 5-(4-Methyl-piperazin-1-yl)pent-2-ynoic acid (4-[{3-chloro-4-fluoro-
 phenyl}amino]pyrido[3,4-d]pyrimidin-6-ylamide, PD0205520, was under
 investigation as a potential inhibitor of the tyrosine kinase (TK)
 activity of the epidermal growth factor receptor (EGFR) for cancer
 treatment. Both radio- and stable-isotope-labeled compds. were required
 for drug absorption, distribution, metabolism and excretion (ADME) and
 quant.
 mass spectrometry bio-anal. studies. PD0205520 ¹⁴C-labeled in the
 pyrimidine ring system was prepared in seven steps in an overall
 radiochem. yield of 26% from [¹⁴C]thiourea. PD0205520 ²H-labeled in the piperazine
 ring was synthesized in four steps in a 32% overall yield.
 IT 877154-66-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of carbon-14- and deuterium-labeled PD0205520)
 RN 877154-66-0 CAPLUS
 CN Piperazine, 1-methyl-, labeled with deuterium (9CI) (CA INDEX NAME)

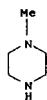


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1989:135210 CAPLUS
 DOCUMENT NUMBER: 110:135210
 TITLE: Synthesis of [³H]clozapine
 AUTHOR(S): De Paulis, Tomas; Davis, Daniel A.; Smith, Howard E.;
 Malarek, David H.; Liebman, Arnold A.
 CORPORATE SOURCE: Dep. Chem., Vanderbilt Univ., Nashville, TN, 37235,
 USA
 SOURCE: Journal of Labelled Compounds and
 (1988), 25(9), 1027-33
 CODEN: JLCRD4; ISSN: 0362-4803
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 110:135210
 AB [³H]clozapine was prepared with a specific activity of 9.9 Ci/mmol by
 an reaction of 8-chloro-11-(methylthio)-5H-dibenzo[b,e][1,4]diazepine with
 excess of [³H]N-methylpiperazine. The latter was prepared from
 N-methylpyrazinium bromide in ethanolic HCl by reduction at room
 temperature with
 tritium over 5% Rh on Al2O3.
 IT 119550-27-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and condensation reaction of, with dibenzodiazepine
 derivative,
 labeled clozapine from)
 RN 119550-27-5 CAPLUS
 CN Piperazine, 1-methyl-, labeled with tritium (9CI) (CA INDEX NAME)



L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1987:597467 CAPLUS
 DOCUMENT NUMBER: 107:197467
 TITLE: Chemistry of nitrogen mustard [2-chloro-N-(2-
 chloroethyl)-N-methylethanamine] studied by nuclear
 magnetic resonance spectroscopy
 AUTHOR(S): Bonding, Bernard T.; Kebbell, Michael J.; Lockhart,
 Ian M.
 CORPORATE SOURCE: Dep. Chem., University of Warwick, Coventry, CV4:7AL,
 UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 2: Physical Organic Chemistry (1972-1999) (1987),
 (6), 705-13
 CODEN: JCPKBB; ISSN: 0300-9580
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 107:197467
 AB MeN(CH₂CH₂X)₂ (I; X = Cl) (II) was converted into the
 N-(2-chloroethyl)-N-
 methylaziridinium ion (III), which was characterized by NMR. Reactions
 of
 II with strong nucleophiles (e.g., S₂O₃²⁻) gave disubstitution products
 (e.g., I; X = S₂O₃²⁻). The intermediacy of III was inferred from the ¹³C
 distribution in product from ¹³C-labeled II. Less reactive nucleophiles
 (e.g., thiourea) yielded disubstitution products via spectroscopically
 detected intermediates III and ClCH₂CH₂NMeCH₂CH₂X (IV; e.g., X =
 SC₂(NH₂)₂). Weaker nucleophiles (e.g., guanosine) did not give
 substitution products. Reaction of II with NH₃ gave a 3-2 ratio of I (X
 = NH₂) and N-methylpiperazine (V). I (X = NH₂) was formed from III, while
 V arose from intramol. cyclocondensation of IV (X = NH₂).
 IT 112023-61-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 112023-61-7 CAPLUS
 CN Piperazine, 1-methyl-, labeled with carbon-13, dihydrochloride (9CI) (CA
 INDEX NAME)



●2 HCl

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=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	16.75	198.66
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.34	-2.34

STN INTERNATIONAL LOGOFF AT 10:51:16 ON 13 JUL 2007